



ARL-RP-0555 • SEP 2015



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REPORT DOCUMENTATION PAGE				Form Approved OMB No. 0704-0188	
<p>Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing the burden, to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number.</p> <p>PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.</p>					
1. REPORT DATE (DD-MM-YYYY)		2. REPORT TYPE		3. DATES COVERED (From - To)	
September 2015		Reprint		January 2014–September 2014	
4. TITLE AND SUBTITLE High Fidelity Simulation of Atomization in Diesel Engine Sprays				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) L Bravo, CB Ivey, D Kim, and ST Bose				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) US Army Research Laboratory ATTN: RDRL-VTP Aberdeen Proving Ground, MD 21005-5066				8. PERFORMING ORGANIZATION REPORT NUMBER ARL-RP-0555	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.					
13. SUPPLEMENTARY NOTES Reprinted from Center for Turbulence Research. [accessed 2015 Sep 14]. https://ctr.stanford.edu/proceedings-2014-summer-program . Proceedings of the 2014 Center for Turbulence Research Summer Program; 2014 August 26; Stanford, CA					
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15. SUBJECT TERMS turbulence, sprays, volume of fluids, CFD, diesel					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			L Bravo
Unclassified	Unclassified	Unclassified	UU	16	19b. TELEPHONE NUMBER (Include area code) 410-278-9525

High fidelity simulation of atomization in diesel engine sprays

By L. Bravo[†], C. B. Ivey, D. Kim[‡], AND S. T. Bose[‡]

A high fidelity numerical simulation of jet breakup and spray formation from a complex diesel fuel injector has been performed. A full understanding of the primary atomization process of diesel fuel injection has not been achieved for several reasons, including the difficulties in accessing the optically dense region. Due to recent advances in numerical methods and computing resources, high fidelity simulations of realistic atomizing flows are currently feasible, providing a new mechanism to study the jet breakdown process. In the present study, a novel volume-of-fluid (VOF) method coupled to a stochastic Lagrangian spray (LSP) model is employed to simulate the atomization process. A common rail fuel injector is modeled by a nozzle geometry provided by the engine combustion network (ECN). The working conditions correspond to a single 90 μm orifice JP-8 fueled injector operating at 90 bar and 373 K and releasing into a 100% nitrogen, 29 bar, 300 K ambient with a $Re_l = 16,071$ and $We_l = 75,334$, putting the spray in the full atomization mode. The experimental dataset from Army Research Lab (ARL) is used for validation and the Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) breakup model (Reitz & Bracco 1979) is used for verification, both in terms of spray angle. Droplet distributions of the simulated spray are provided for future experimental comparisons and secondary atomization simulations using LSP modeling.

1. Introduction

To date, one of the main bottlenecks in engineering spray modeling of combustion systems is an accurate description of the primary atomization process. Several contemporary numerical solvers adopt coarse approximations in the dense region based on injecting nozzle-sized particles subject to Kelvin-Helmholtz type instabilities coupled with Lagrangian particle tracking techniques (Som & Aggarwal 2009; Senecal 2012). Significant success has been achieved with these methods; however, they require a posteriori knowledge of the spray process to calibrate the model, making an a priori investigation impossible. Historically, the advancement of primary atomization models has been hindered by the well-known difficulties in measuring the optically dense spray region. Although experimentalists have had success with modern methods, such as ballistic imaging and x-ray techniques, extraction of full four dimensional information with sufficient spatial and temporal resolution for a detailed analysis is still infeasible (Linne *et al.* 2006; Wang *et al.* 2006; Coletti *et al.* 2014).

Remarkable progress has been made in recent years in the development of robust numerical methods for handling interfaces, enabling researchers to perform highly resolved simulations of multiphase flow (Gorokhovski & Herrmann 2008). Desjardins reported on the development of the level set/ghost fluid method utilizing high order schemes to

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study multiphase flows (Desjardins *et al.* 2008). The accuracy of the numerical technique was corroborated through several studies, including the atomization of a liquid diesel jet at moderately low Reynolds number, $Re = 3000$. In a related study, Desjardins conducted *detailed* numerical simulations (DNS) of primary atomization for several values of Reynolds and Weber numbers ($2000 < Re < 3000$, $500 < We < 2000$), reporting on velocity statistics across the turbulent jet (Desjardins & Pitsch 2010). More recently, using a refined level set grid approach, Herrmann discussed the impact of finite grid resolution on the phase interface geometry of the liquid jet core under diesel engine conditions with $Re = 5000$ and an injection velocity of 100 m/s (Herrmann 2011). In this work, it was reported that turbulence is the driving mechanism of atomization within the first 20 diameters downstream of the injector. It was also determined that 6 grid points are needed to obtain grid-independence of larger scale drops. These studies provide a critical database to drive the next-generation spray model development. Note that, as with most other DNS studies, no quantitative comparison to experimental data is typically provided.

The need to accurately model two phase atomizing flows in high speed jets is particularly important in diesel injectors where the quality of the fuel and oxidizer mixing is essential for lean combustion. Fuel/air mixture formation is also a very important factor in increasing engine efficiencies and power densities. Spray and atomization characteristics have to be considered to optimize the design of the combustion chamber to reduce exhaust emissions and to improve combustion performance. Also, diesel spray characteristics can be influenced by the injector geometry, the injection parameters, and the flow mixing inside the combustion chamber. Therefore, simulations should account for system level complexities, including real injector features to accurately predict realistic spray dynamics.

Additionally, the computational expense of resolving all the critical length scales at large Weber number is prohibitively large, so the application of DNS to simulate realistic diesel injector conditions has been severely limited. A liquid jet moving with an $\mathcal{O}(100)$ m/s relative velocity with respect to the quiescent gas can generate droplets with diameters as small as a few microns (Desjardins & Pitsch 2010). Hence, there is a need to develop more accurate engineering breakup spray models for the primary and secondary breakup modes to reduce the computational cost when simulating a spray filled domain.

The objective of the current work is to investigate the atomization behavior of a high-speed single hole jet with complex internal geometry. A novel unstructured volume-of-fluid (VOF) method has been adopted, which is geometric and un-split, enforcing exact mass conservation on an unstructured grid (Kim *et al.* 2013, 2014). In this study, the VOF method is coupled to the Lagrangian spray (LSP) framework to increase the computational efficiency and to apply sub-grid atomization models. Hence, the phase interface resolved by the grid is captured by the VOF method, while the under resolved small scale droplets are transferred from the VOF interface representation to the LSP particle tracking and further breakup is handled by a stochastic breakup model. Measurements were conducted at the Spray and Combustion Research Facility of the Army Research Lab (ARL) to qualitatively complement the simulation and to validate the simulation in terms spray angle. The Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) breakup model (Reitz & Bracco 1979) is used to verify the simulation in terms of spray angle. Droplet distributions were generated for future experimental comparisons and secondary atomization models.

2. Methods

2.1. Simulation

The detailed numerical simulation of the interface was performed using a novel geometric unsplit VOF method that is conservative on unstructured meshes coupled to a stochastic Lagrangian spray (LSP) framework. The geometric VOF method ensures discrete conservation and boundedness of the volume fraction, F , by utilizing non-overlapping flux polyhedra for donor volumes (see Ivey & Moin 2012 for a description of flux polyhedra). The volume-of-fluid method uses piecewise linear interface calculation (PLIC) representation of the interface, requiring an interface normal, \hat{n} . \hat{n} is calculated from an auxiliary level set, G , that was updated using the geometric advection algorithm to keep it consistent with F . Curvature, κ is also calculated from the G using the *direct front curvature* method (Herrmann 2006). After \hat{n} and κ are calculated, G is reconstructed to strictly follow the PLIC representation using a bisection algorithm to calculate the local G field (to enforce F) and the reconstructed distance function (Cummins *et al.* 2005) method to propagate the G field throughout the band. For consistency (and stability), mass and momentum are convected using the geometric VOF method. To diminish the strict over-flow time step requirements on VOF schemes, multiple *frozen* velocity advection updates (taken as 3 here) are performed for each momentum step. Several validation studies have been performed that tested the numerical accuracy and robustness of the solver (Kim *et al.* 2013, 2014).

For computational efficiency, the VOF representation is coupled to a stochastic Lagrangian spray (LSP) representation. Interfacial features are characterized by contiguous regions of $F > 0$. Under resolved (taken $< 5^3$ cells here) interfacial flow structures are replaced by a spherical droplet of equal volume. No additional breakup model is employed here so as to capture the instabilities leading to atomization directly. LSP droplets follow particle drag laws and a stochastic breakup model based on critical Webber number (Ham *et al.* 2003).

The simulation was conducted on the nozzle geometry available through the engineer combustion network (ECN) with flow conditions corresponding to an injection pressure of 90 bar, a background pressure of 20 bar, and a bulk jet exit velocity of 127 m/s. The Reynolds and Weber number were calculated with JP-8 fuel properties database (at 373 K) and yielded a value of $Re_l = 16,071$ and $We_l = 75,334$. The critical length scales, determined from the problem configuration, range from the nozzle orifice integral scale ($l_i = d = 90 \mu\text{m}$), to the viscous scale ($0.09 \mu\text{m}$), and down to Kolmogorov critical radius ($0.2 \mu\text{m}$). The pipe flow viscous scale and the critical radius are defined as,

$$l_v = 1/0.2Re^{-7/8} \quad \text{and} \quad l_{cr} = \left(\frac{\sigma^3}{\rho^3 \epsilon^2} \right)^{1/5}. \quad (2.1)$$

A large eddy simulation dynamic Smagorinsky model was adopted to treat the smallest flow structures and for computational efficiency. In the nozzle, a wall resolved approach was utilized with $\Delta x^+, \Delta y^+ \sim 1$ near the wall (calculated from l_v), $\Delta x^+, \Delta y^+ \sim 50$ near the center, and $\Delta z^+ \sim 70$ (see Figure 1). The mesh refinement is cartesian in nature, forcing $\Delta x = \Delta y = \Delta r$. A mesh of ~ 60 million hexahedral control volumes was used to discretize the domain. Mesh points were concentrated in the jet spray envelope to resolve the interface, while coarse buffer regions were added in the radial and axial regions in order to reduce the impact of the boundary conditions (see Figure 2). Within the spray envelope, $\Delta/l_{cr} \sim 0.5$ near the unperturbed nominal interface to capture the instabilities and $\Delta/l_{cr} \sim 40$ throughout the rest of the spray envelope to leverage the LSP framework

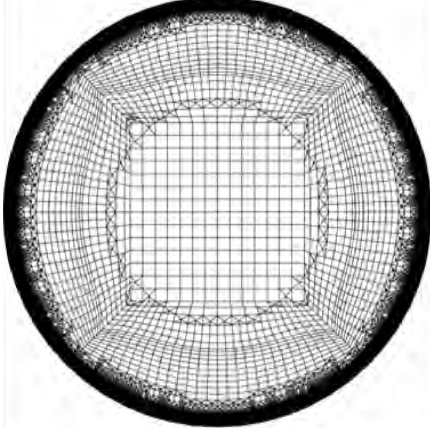


FIGURE 1. Mesh slice at nozzle exit.

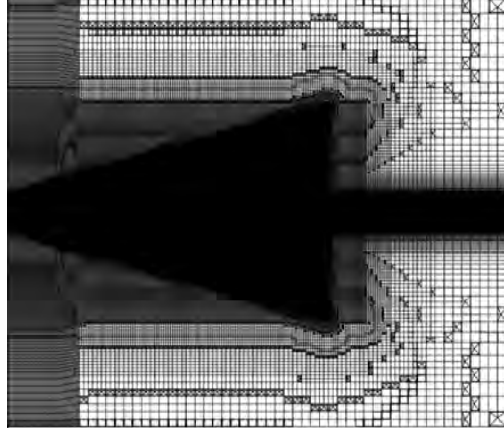


FIGURE 2. Mesh slice through jet centerline.

for savings. The numerical boundary conditions in the ambient region were a constant inflow set to 5% the bulk jet velocity, a slip condition over the radial boundaries, and a uniform outflow.

2.2. Experiment

The experiments in this study were conducted at the Army Research Laboratory by injecting a high speed JP-8 fueled spray into a high temperature pressure (HTPV) flow through chamber. The HTPV is designed to reach a maximum pressure of 150 bar and a maximum temperature of 1000 K using a BOSCH common rail injection system for precise fuel delivery (Kurmann *et al.* 2014). The vessel is equipped with closed loop control for pressure and temperature. The flow through chamber is held constant at 58 m³/hr. An on-site nitrogen generator produced the necessary nitrogen for testing, which was maintained at 99% purity during experiments. To allow for optical access, the vessel is outfitted with 3 fused silica windows with dimensions of 147 mm diameter by 85 mm thickness. To protect the 85 mm thick pressure windows from fuel contamination, 6 mm thick fused silica windows are placed between the 85 mm windows and the spray zone.

High speed near field spray region images were acquired using a single LED light source and a Photron SA5 camera operating at 90,000 fps for line of sight measurements. For the experiments presented, image size was set to 320 by 192 pixels and the corresponding scaling was 5.6 $\mu\text{m}/\text{pixel}$. Chamber conditions were set to 20 bar and 300K prescribing a density ratio of 34 kg/m³. Fuel injection pressure was set to 90 bar with a 3 ms injection duration, and a total of 2.2 mg of injected mass was measured via an IAV injection analyzer. Figures 3 and 4 show two instances where the spray behavior goes from transitional to fully atomizing mode.

2.3. Theory

Reitz dispersion model has been proposed to study the spray angle by employing aerodynamic arguments (Reitz & Bracco 1979). It includes the ratio of the Reynolds and Weber number of the liquid flow in the function $f(\gamma)$ and it is written as

$$\tan(\theta) = \frac{4\pi}{A} \left(\frac{\rho_g}{\rho_l} \right) f(\gamma), \quad (2.2)$$

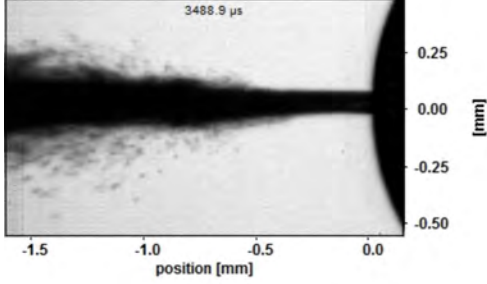


FIGURE 3. High speed near field image of JP-8 spray during transition state

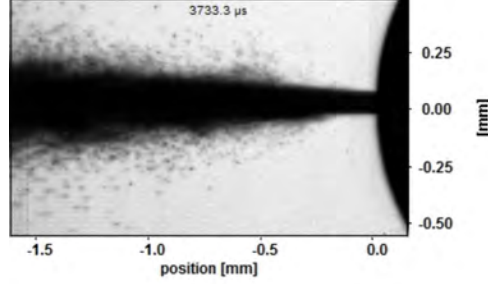


FIGURE 4. High speed near field image of JP-8 spray during fully atomized state



FIGURE 5. Q criterion isosurface colored by streamwise velocity in the diesel spray injector as viewed from the nozzle exit.



FIGURE 6. U contour slice at jet centerline.

where ρ_g and ρ_l are the liquid and gas density, and A is a constant that depends on the nozzle design, $A = 3.0 + 0.28l_0/d_0$, with d_0 is the nozzle diameter and l_0 is the length of the nozzle hole. The parameter $f(\gamma)$ is function of the physical properties of the liquid and injection velocity and defined as, $f(\gamma) = \sqrt{3}/6[1 - \exp(-10\gamma)]$ with $\gamma = (Re_l/We_l)^2 \rho_l/\rho_g$ where the injection velocity is based on Bernoulli arguments, $V_{inj} = C_v \sqrt{2\Delta P/\rho}$.

3. Results

The nozzle flow turbulence was visualized by sampling the velocity flow-field and using the classical Q criterion defined as $Q = 1/2(\|\Omega_{ij}\| - \|S_{ij}\|)$ and colored by the streamwise velocity component, U (see Figure 5). The Q criterion isosurface shows hairpin vortex structures arising from the interaction of the fluid with the wall, having peak streamwise velocity magnitudes towards the center of the pipe flow. The vortex structures are irregular as compared to a traditional pipe flow; this discrepancy can be explained by the favorable pressure gradient of the nozzle and the lack of perfect symmetry in the experimentally modeled geometry. Nevertheless, the emerging flow field can be characterized as turbulent and the resultant jet breakdown can be interpreted as being in the spray atomization regime. The turbulent inflow combined with the jet instabilities lead to the



FIGURE 7. F isosurface and Lagrangian particles alongside the diesel spray injector.

chaotic jet behavior illustrated by the streamwise velocity contour in Figure 6.

Figure 7 shows the spray formation process at steady full atomization conditions as visualized using the $F = 0.5$ isosurface and the LSP tracked droplets with reference to the nozzle geometry. Note the growth of the hydrodynamics instabilities and the resultant spray cone. The present simulation solely models the static fully opened valve configuration.

Figures 8-11 show the radial variations of U and F statistics with axial distance. Figure 8 shows the use of 5% co-flow field used to stabilize the solution ($\bar{U} \neq 0 \forall r > D/2$) and the experimental bulk velocity (at $0 D$). Indicative of growing jets, the \bar{U} profiles broaden downstream. Figure 9 shows the mean F distribution, which includes the equivalent volume fraction of the Lagrangian particles. As in \bar{U} , but to a smaller degree, \bar{F} profiles broaden downstream. The \bar{F} profiles decrease in height downstream demonstrating the breakdown and fluctuation of the liquid jet. Note that the dispersion characteristics between velocity and volume fraction fields are quite different, demonstrating the entrainment effect on the velocity fields and the conservation of mass of the volume fraction fields. The turbulent kinetic energy (TKE) radial profiles are shown in Figure 10. The nozzle pipe flow injects sharp TKE peaks, generating turbulent structures at fluid interface. The TKE facilitates the jet breakdown and grows with the shear layer.

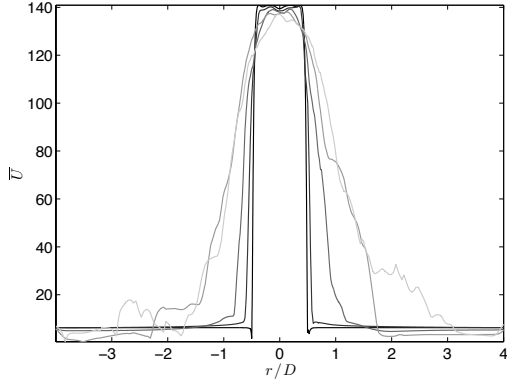


FIGURE 8. Mean streamwise velocity as a function of radius for 5 downstream stations: $z/D = \{0, 4, 8, 12, 16\}$ (dark to light).

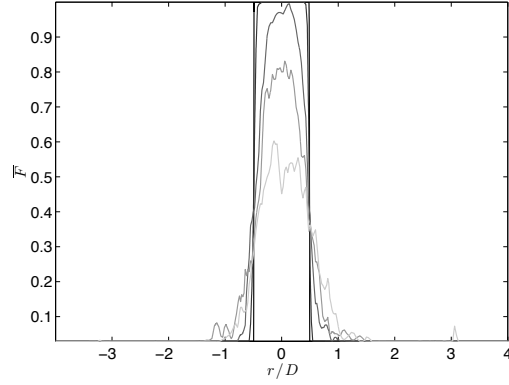


FIGURE 9. Mean volume fraction (including Lagrangian spray) as a function of radius for 5 downstream stations: $z/D = \{0, 4, 8, 12, 16\}$ (dark to light).

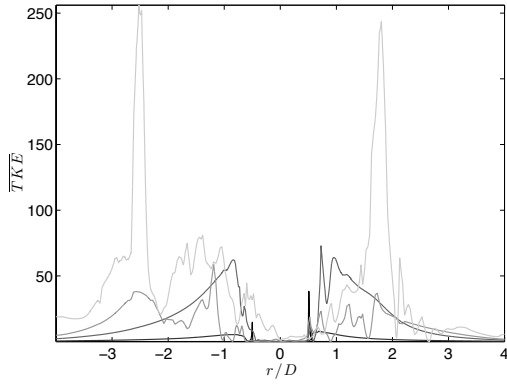


FIGURE 10. Mean turbulent kinetic energy as a function of radius for 5 downstream stations: $z/D = \{0, 4, 8, 12, 16\}$ (dark to light).

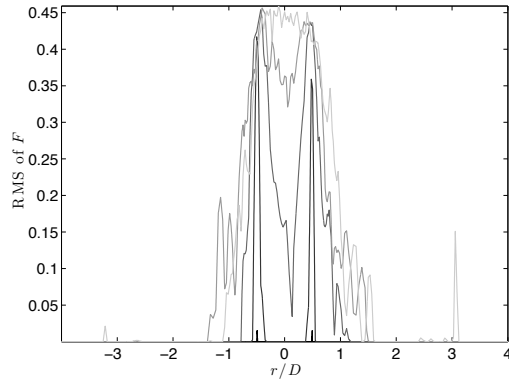


FIGURE 11. Root mean square of volume fraction (including Lagrangian spray) as a function of radius for 5 downstream stations: $z/D = \{0, 4, 8, 12, 16\}$ (dark to light).

The intensity, F root mean square (RMS) profiles, in Figure 11 shows the intensity fields increasing with the growth of the shear growth layer.

The statistics have not fully converged, as shown in the Figure 8, so in order to extract a preliminary estimate of the spray angle, θ , we fit a Gaussian curve to each of the mean velocity profiles. Figure 12 shows the Gaussian fits, which are not centered at the origin, evidencing the lack of axisymmetry of the real geometry (the spray comes off at an angle). The full width half maximum (FWHM) of the Gaussian fits to the mean streamwise profiles is shown in Figure 13; the change of the linear fit to the FWHM with axial distance provides the spray angle, θ .

The experimental spray angle was determined via line of sight observations of 200 spray images (sampling frequency of $11.1 \mu\text{s}$) while tracking the interface of the jet core region with respect to the jet centerline. The total sampling time corresponds to 2.2 ms in the full atomization spray mode ($Re = 16,071$ and $Oh = 0.017$). The initial transients were not included in the procedure for consistency with the simulation results. The spray

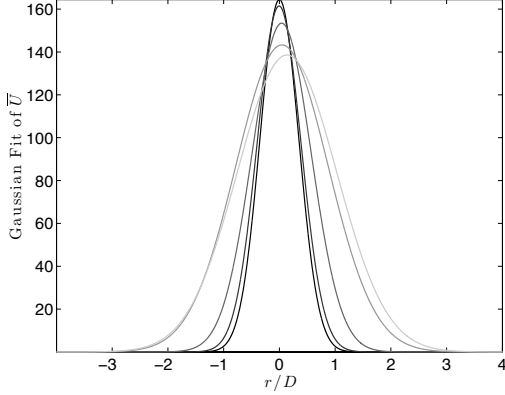


FIGURE 12. Gaussian fit to mean streamwise velocity as a function of radius for 5 downstream stations: $z/D = \{0, 4, 8, 12, 16\}$ (dark to light).

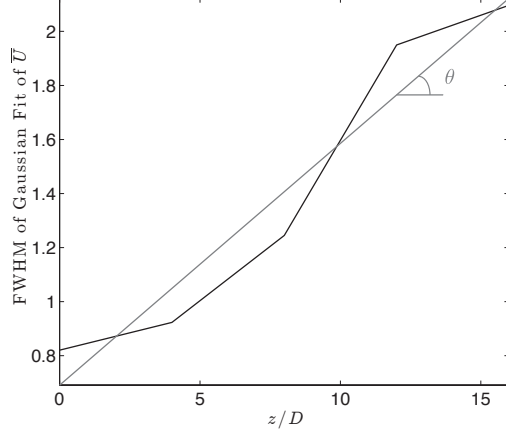


FIGURE 13. Full width half maximum of gaussian fit to mean stream wise velocity as a function of downstream location. θ is the angle of linear fit to the full width half maximum (shown in gray).

angles extracted from Reitz theory, simulation, and experiment are respectively

$$\theta_{\text{Reitz}} = 5.8325^\circ, \quad \theta_{\text{sim}} = 5.1125^\circ \quad \text{and} \quad \theta_{\text{exp}} \sim 4^\circ. \quad (3.1)$$

The simulation and theoretical dispersion results appear to be in good agreement. However, there is a 1° discrepancy with the experiments featuring a spray angle of 4° . The differences can be in part due to variations in the nozzle orifice diameter and nozzle shape that arise from manufacturer fabrication eccentricities. This has been reported in the literature previously for ECN type injectors where geometric inconsistencies were thoroughly reported (Kastengran *et al.* 2012). The impact of these discrepancies can clearly affect the spray parameters.

Secondary atomization models require an initial droplet spray profile, parameterized by droplet diameter and distance away from jet. Droplet sizes and counts are calculated from the combination of the LSP particles and the resolved VOF features (calculated using the same method to transfer from VOF to LSP for under resolved features, but with a larger domain cell count). Figure 14 shows the average number of droplets for a given droplet diameter. The droplets range from approximately $1 - 10 \mu\text{m}$, the average droplet diameter is $2.9786 \mu\text{m}$, and the most likely droplet diameter is $1.5055 \mu\text{m}$. Droplet diameters $< 1 \mu\text{m}$ were spontaneously evaporated and were not tracked. Figure 15 shows the average droplet diameter at a given distance away from the jet center. The average droplet size increases away from the jet going from approximately $2 - 7 \mu\text{m}$.

4. Conclusions

In this investigation a high fidelity simulation approach was adopted to study the atomization physics of a diesel injector with detailed nozzle internal geometry. The nozzle flow field was characterized through visualizations of Q isosurfaces for turbulence patterns. The complexity of the geometry and system dynamics was characterized by a snapshot of the volume fraction isosurface and Lagrangian droplets. Also, mean streamwise velocity and volume fraction statistics show the structure of the high speed jet. The turbulent

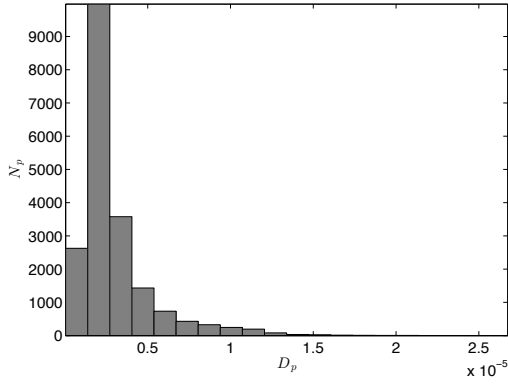


FIGURE 14. Number of droplets as a function of diameter

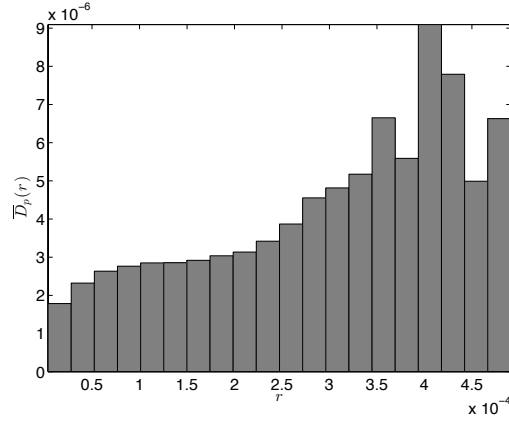


FIGURE 15. Mean droplet diameter as a function of radius

kinetic energy and volume fraction intensity profiles characterize the interfacial mixing processes. Comparison with Reitz spray theory and ARL measurements of the near nozzle flow field show that the simulation captures the correct dispersion characteristics. The spray was further characterized using droplet size and spatial distribution plots. Further work is presently on the way, using higher resolution to establish numerical convergence and to capture the hydrodynamic flow instabilities for comparison with classical instability models.

Acknowledgments

The authors acknowledge the following award for providing {computing, visualization} resources that have contributed to the research results reported within this report: MRI-R2: Acquisition of a Hybrid CPU/GPU and Visualization Cluster for Multidisciplinary Studies in Transport Physics with Uncertainty Quantification (<http://www.nsf.gov/awardsearch/showAward.do?AwardNumber=0960306>). This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

This research was supported in part by an appointment to the U.S. Army Research Laboratory Postdoctoral Fellowship Program administered by the Oak Ridge Associated Universities through a contract with ARL.

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